Non-intrusive Termination of Noisy Optimization

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Problem Setting

When should you terminate algorithms solving

$$\min_x f(x) : \mathbb{R}^n \to \mathbb{R}$$

when f is

- Computationally expensive
- There is noise in the computation of f

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Practitioners typically stop the optimization when:

- A measure of criticality is satisfied (e.g., gradient norm, mesh size)
- The computational budget is satisfied (e.g., number of evaluations, wall clock time)

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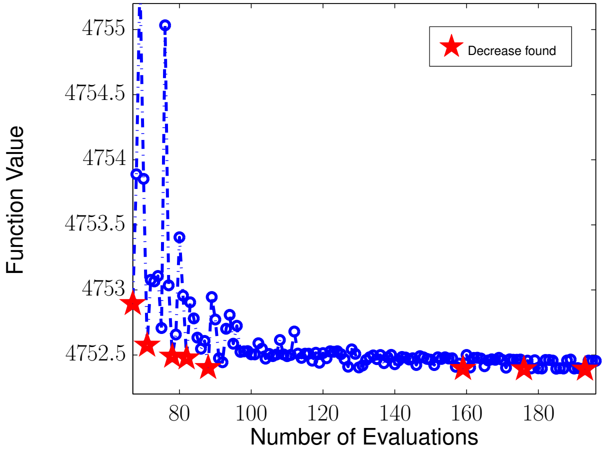
Definition

This is an attempt to solve the true problem:

$$\begin{array}{ll} \min\limits_{t} & \text{Computational expense}(t) \\ \text{s.t.} & \text{Acceptable accuracy of the solution}(t), \end{array}$$

Example from Nuclear Physics



Quotes

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Modifications for Noisy Function

1. Functions with stochastic noise, $\mathrm{Var}\{f(x)\} > 0$,
   - UOBYQA, DIRECT, and Nelder-Mead methods have all been modified in the literature to repeatedly sample points.
   - Some adjust the maximum number of replications based on the noise level.
   - Termination was still based on traditional measures:
     - points clustered together
     - no decrease in the best function value

2. Functions with deterministic noise, (iterative methods, round-off error)
   - Kelley- proposes a restart technique for Nelder-Mead when low-level noise is present, but terminates independent of the noise.
   - Gramacy et al. - stops a treed Gaussian process when the maximum improvement statistic is sufficiently small.
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Desirable Test Properties

For a sequence of points and function values

$$\{x_1, \cdots, x_m\} \subseteq \mathbb{R}^n, \{f_1, \cdots, f_m\} \in \mathbb{R}, \mathcal{F}_i = \{(x_1, f_1), \cdots, (x_i, f_i)\}$$

produced by a local minimization solver, it is preferable if the termination test is:

- Algorithm independent
  - Uses only the x_i and f_i.
- Shift and scale invariant in f
  - Stops sequences $\{f_i\}$ and $\{\alpha f_i + \beta\}$ at the same point.

Useful notation: Let $f_i^* = \min_{1 \le j \le i} \{f_j\}$ and x_i^* be the corresponding point.

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Estimate of the Noise Level

Let $\hat{\varepsilon}_{i_r}$ be the relative noise in f_i.

For stochastic noise, $\hat{\varepsilon}_{i_r} = \dfrac{\sqrt{\mathrm{Var}\{f(x_i)\}}}{E\{|f(x_i)|\}}$, in which case, for $\alpha > 0$:

$$\hat{\varepsilon}_{i_r} = \frac{\alpha\sqrt{\mathrm{Var}\left\{f(x_i)\right\}}}{\alpha E\left\{|f(x_i)|\right\}} = \frac{\sqrt{\alpha^2\mathrm{Var}\left\{f(x_i)\right\}}}{\alpha E\left\{|f(x_i)|\right\}} = \frac{\sqrt{\mathrm{Var}\left\{\alpha f(x_i)\right\}}}{E\left\{|\alpha f(x_i)|\right\}}.$$

$\hat{\varepsilon}_{i_r}$ is scale invariant.

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$\hat{\varepsilon}_{i_r} E\left\{|f(x_i)|\right\}$ is shift invariant.

For deterministic noise, invariance depends on the methods used to obtain $\hat{\varepsilon}_{i_r}$ and $\hat{\varepsilon}_{i_r}|f_i|$. For one such method, see Moré & Wild (2011).

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Tests on Function Values, ϕ_1

For $\nu_{\mathcal{F}_i}, \mu \in \mathbb{R}_+,\ \kappa \in \mathbb{N}$. Let $\hat{\varepsilon}_{i_r}$ be an estimate for the relative noise level of f_i.

$$\phi_1\left(\mathcal{F}_i; \nu_{\mathcal{F}_i}, \kappa, \mu\right) \text{ stops when } \frac{f^*_{i-\kappa+1} - f^*_i}{\kappa} \le \mu \left|f^*_i\right| \nu_{\mathcal{F}_i}$$

- If $\nu_{\mathcal{F}_i} = 1$: stop when the average relative change in the best function value over the last κ evaluations is less than μ. (scale invariant)
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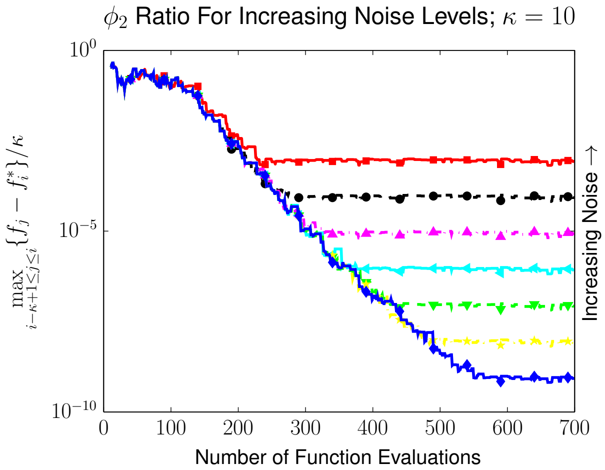
Dependence on the Noise Level



Tests on x Values

For $\mu \in \mathbb{R}_+$, $\kappa \in \mathbb{N}$.

- $\phi_3(\mathcal{F}_i; \kappa, \mu)$ stops when $\max_{i-\kappa+1 \leq j,k \leq i} \|x_j - x_k\| \leq \mu$
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Comparison Test

As a point of comparison, we define the test

- $\phi_5(\mathcal{F}_i; \kappa)$ to stop after κ iterations

This test is trivially shift and scale invariant.

Problem Set

53 problems of the form:

$$f(x) = 1 + (1 + \sigma g(x)) \sum_{i=1}^{m} F_i^s(x)^2,$$

- For stochastic noise

$$\mathrm{Var}\left\{g(x)\right\} = 1$$

- For deterministic noise

$$g(x) = \xi(x)(4\xi(x)^2 - 3))$$

$$\xi(x) = 0.9 \sin(100\|x\|_1) \cos(100\|x\|_\infty) + 0.1 \cos(\|x\|_2).$$

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We have 6 algorithms from the following classes:

1. Nelder-Mead implementations
2. Pattern search methods
3. Model-based methods
4. . . . and methods which cross these classes

that we ran on all 53 problems, leaving us with 318 algorithm runs to form $\mathcal{P}$.

For each termination test t and $p \in \mathcal{P}$, let

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Measures of Quality in a Stopping Point

- Accuracy: How far from the best point does the test stop?

$$\frac{f^*_{i^*_{p,t}} - f^*_{i_{\max}}}{f^*_{i^*_{p,t}}} \quad \text{if} \quad i^*_{p,t} < i_{\max}$$

- Performance: Could the test have stopped sooner?

  Given a collection of tests $\mathcal{T}$, what $t \in \mathcal{T}$ stops when

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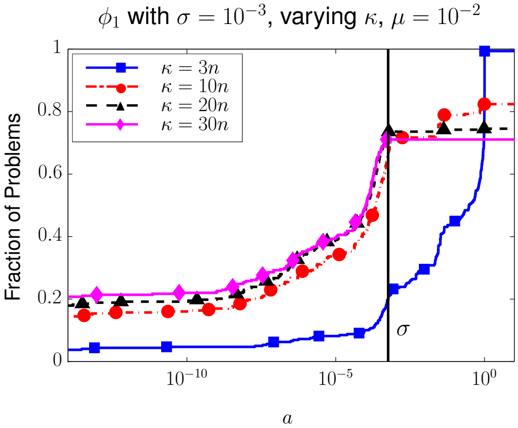
Accuracy Profiles



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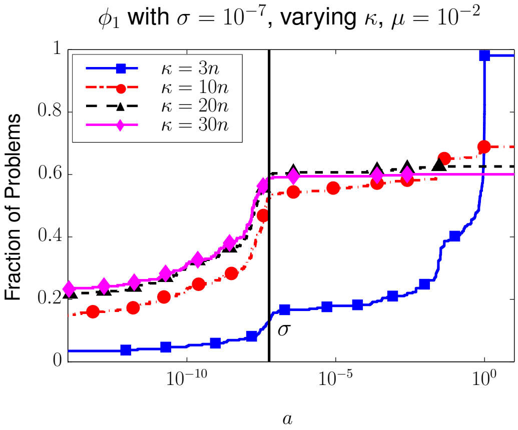

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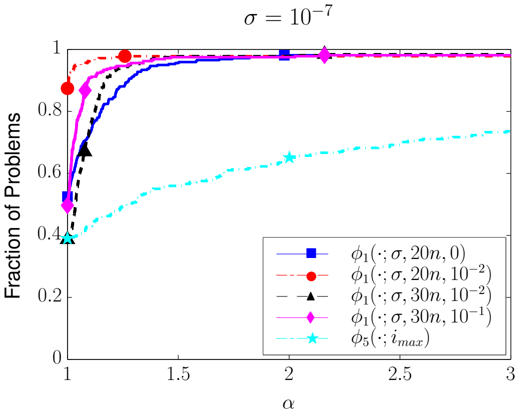

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Other test

We performed similar analysis on the other families of tests and found the best:

- $\phi_1(\cdot, \cdot, 20n, 10^{-2})$ Stop when
$$\frac{f^*_{i-\kappa+1} - f^*_i}{20n} \leq 0.01 \left| f^*_i \right| \hat{\varepsilon}_{i_r}$$
- $\phi_2(\cdot, \cdot, 10n, 10)$ Stop when
$$\max_{i-10n+1 \leq j \leq i} \left| f_j - f^*_i \right| \leq 10 \left| f^*_i \right| \hat{\varepsilon}_{i_r}$$
- $\phi_3(\cdot, n, 10^{-7})$ Stop when
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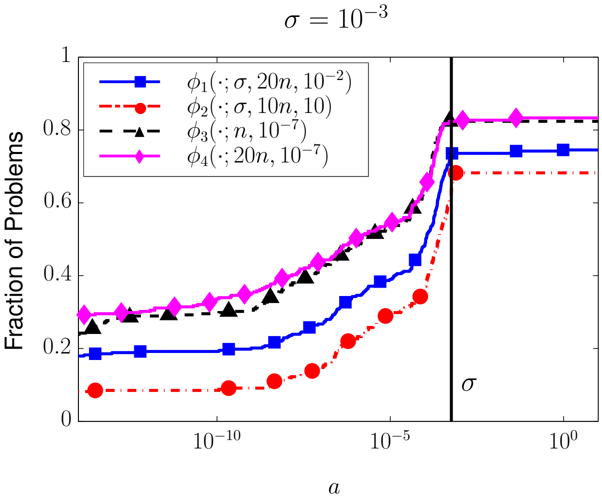
Most Accurate Tests



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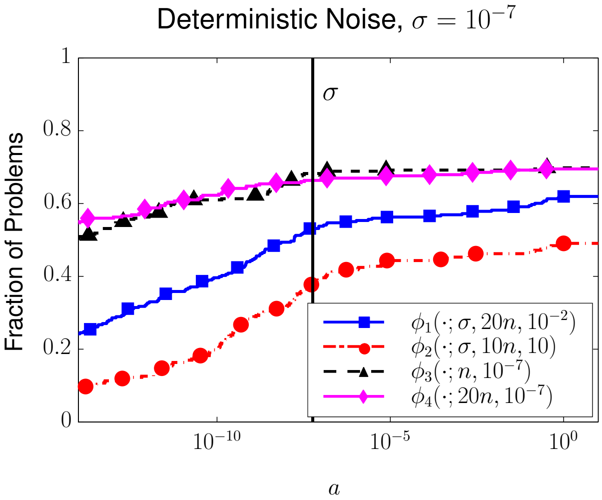
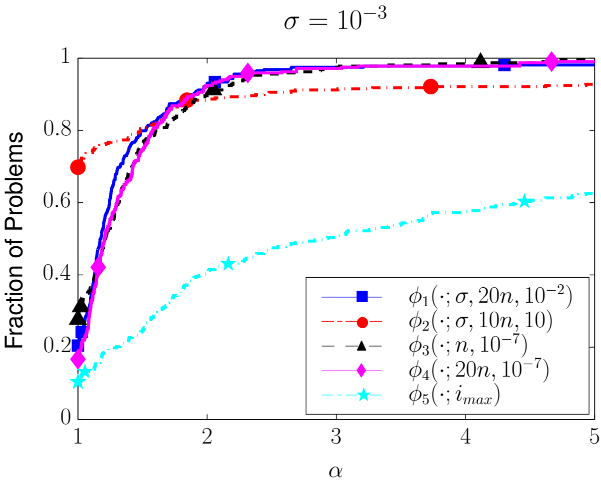


Performance Profiles for Most Accurate Tests



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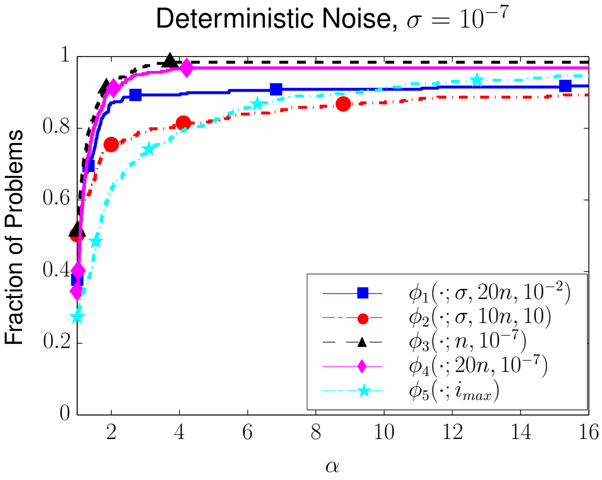

Recommendations for termination tests

Test	κ	μ	Interpretation of Stopping Rule
ϕ_1	$\approx 20n$	≈ 0.01	Stop when the average relative decrease in the best function value over the last $20n$ function evaluations is less than one-hundredth of the relative noise level.
ϕ_2	$\approx 10n$	≈ 10	Stop when the last $10n$ function evaluations are within 10 times the absolute noise level of the best function value.
ϕ_3	$\approx n$	$\approx 10^{-7}$	Stop when the last n points evaluated are within a distance of 10^{-7} of each other.
ϕ_4	$\approx 20n$	$\approx 10^{-7}$	Stop when the best point hasn't moved more a distance of 10^{-7} for $20n$ evaluations.

Final Comments:

- Tests using knowledge of the noise are better, especially as the noise level increases.

- It is likely a better use of a computational budget to restart a stagnant algorithm.

- Nothing in these tests prevent their inclusion in
  - Derivative-based algorithms
  - The refinement stage of global algorithms

- For further information, see:

  `http://www.mcs.anl.gov/~wild/tnoise`